Chapter 3

Rotations

3.1 Rotation operators

Consider two Cartesian coordinate systems C and C' that share the same origin but are rotated with respect to each other. If one want to rotate C into C', three successive rotations are usually needed. With the Euler angles $\omega = \alpha\beta\gamma$, the three rotations can be defined as

i) Rotate C by γ about its z-axis
ii) Rotate C by β about its y-axis (*i.e.* about the original y-axis)
iii) Rotate C by α about its z-axis, (*i.e.* the same axis as in i)),

or in terms rotation matrices

$$\begin{pmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \times$$
$$\begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} \tag{3.1}$$

To derive an expression for the rotation operator $D(\omega)$ we recall the definition $L = -i\hbar r \times \nabla$. Expressing L in spherical coordinates we get

$$\begin{aligned} L_x &= i\hbar(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}) \\ L_y &= i\hbar(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}) \\ L_z &= -i\hbar\frac{\partial}{\partial\varphi} \end{aligned} \tag{3.2}$$

For a small rotation of an arbitrary function $f(\bar{r})$ around the z-axis we obtain

$$D_z(\Delta\varphi)f(\bar{r}) = f(r,\theta,\varphi-\Delta\varphi) = f(r,\theta,\varphi)\underbrace{-\Delta\varphi\frac{\partial}{\partial\varphi}}_{-i/\hbar\Delta\varphi L_z} f + O(\Delta\varphi)^2 \tag{3.3}$$

and

$$D_z(\Delta\varphi) = 1 - \frac{i}{\hbar}\Delta\varphi L_z + O(\Delta\varphi)^2 \tag{3.4}$$

Performing n successive infinitesimal rotations, letting $n \to \infty$ and $\Delta\varphi \to 0$, we get using Eq. (3.4)

$$D_z(\theta)f = \lim_{\Delta\varphi\to 0, n\to\infty, n\Delta\varphi=\theta}(1 - \frac{i}{\hbar}\frac{\theta}{n}L_z + O(\frac{\theta}{n})^2)^n f = \sum_{k=0}^{\infty}\frac{(-\frac{i}{\hbar}\theta L_z)^k}{k!}f = \exp(-\frac{i}{\hbar}\theta L_z)f \tag{3.5}$$

Because the function $f(\bar{r})$ is an arbitrary function we have the following relation

$$D_z(\theta) = \sum_{k=0}^{\infty}\frac{(-\frac{i}{\hbar}\theta L_z)^k}{k!} = \exp(-\frac{i}{\hbar}\theta L_z) \tag{3.6}$$

Interestingly enough we will now see that Eq. (3.6) leads to the commutation relations $[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$. To show this we recall the rotation matrices and consider the infinitesimal rotation ϵ

$$R_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{3.7}$$

Expanding to $O(\epsilon^3)$

$$R_z(\epsilon) = \begin{pmatrix} 1-\epsilon^2/2 & -\epsilon & 0 \\ \epsilon & 1-\epsilon^2/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} + O(\epsilon^3) \tag{3.8}$$

$$R_y(\epsilon) = \begin{pmatrix} 1-\epsilon^2/2 & 0 & \epsilon \\ 0 & 1 & 0 \\ -\epsilon & 0 & 1-\epsilon^2/2 \end{pmatrix} + O(\epsilon^3) \tag{3.9}$$

$$R_x(\epsilon) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\epsilon^2/2 & -\epsilon \\ 0 & \epsilon & 1-\epsilon^2/2 \end{pmatrix} + O(\epsilon^3) \tag{3.10}$$

Forming

$$R_x(\epsilon)R_y(\epsilon) - R_y(\epsilon)R_x(\epsilon) = \begin{pmatrix} 0 & -\epsilon^2 & 0 \\ \epsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = R_z(\epsilon^2) - 1 \tag{3.11}$$

Eq. (3.11) tells us how the commutation relations look for rotations about different axis. The operator analogue to Eq. (3.11) is , using Eq. (3.6) and expanding to $O(\epsilon^3)$

$$\begin{aligned}&\left(1 - iL_x\epsilon/\hbar - L_x^2\epsilon^2/\hbar^2 + O(\epsilon^3)\right)\left(1 - iL_y\epsilon/\hbar - L_y^2\epsilon^2/\hbar^2 + O(\epsilon^3)\right) - \\ &\left(1 - iL_y\epsilon/\hbar - L_y^2\epsilon^2/\hbar^2 + O(\epsilon^3)\right)\left(1 - iL_x\epsilon/\hbar - L_x^2\epsilon^2/\hbar^2 + O(\epsilon^3)\right) = \\ &1 - iL_z\epsilon^2/\hbar + O(\epsilon^3) - 1\end{aligned} \tag{3.12}$$

This expression easily simplifies to

$$[L_x, L_y] = i\hbar L_z \tag{3.13}$$

or

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \tag{3.14}$$

Eq. (3.6) resulted in the commutation relations Eq. (3.14) and it is therefore safe to use the more general definition

$$D_z(\theta) = \exp(-\frac{i}{\hbar}\theta J_z) \tag{3.15}$$

$|jm\rangle$ is an eigenket to J_z with eigenvalue $m\hbar$, thus

$$D_z(\theta)|jm\rangle = \sum_{k=0}^{\infty}\frac{(-\frac{i}{\hbar}\theta J_z)^k}{k!}|jm\rangle = \sum_{k=0}^{\infty}\frac{(-i\theta m)^k}{k!}|jm\rangle = \exp(-i\theta m)|jm\rangle \tag{3.16}$$

We conclude

$$D(\omega) = \exp(-\frac{i\alpha}{\hbar}J_z)\exp(-\frac{i\beta}{\hbar}J_y)\exp(-\frac{i\gamma}{\hbar}J_z) \tag{3.17}$$

3.2 Matrix elements of finite rotation operators

The representation matrix of an operator α is defined as

$$\alpha|A\rangle = \sum_B |B\rangle\langle B|\alpha|A\rangle \tag{3.18}$$

$|A\rangle$ are the orthonormal eigenkets for the representation. Eq. (3.18) gives for the general rotation of an angular momentum eigenfunction

$$D(\omega)|jm\rangle = \sum_{j'm'}|j'm'\rangle\langle j'm'|D(\omega)|jm\rangle \tag{3.19}$$

where the matrix elements are written

$$D^{(j'j)}_{m'm}(\omega) = \langle j'm'|D(\omega)|jm\rangle \tag{3.20}$$

Because $D(\omega)$ only change the m quantum number j is always unchanged and Eq. (3.20) is written $D^{(j)}_{m'm}(\omega)$

Example: Construct $D^{(1/2)}_{m'm}(\alpha\beta\gamma)$.

$$\begin{aligned} D^{(1/2)}_{m'm} &= \langle jm'|\exp(-\frac{i\alpha}{\hbar}J_z)\exp(-\frac{i\beta}{\hbar}J_y)\exp(-\frac{i\gamma}{\hbar}J_z)|jm\rangle \\ &= \exp(-i\alpha m')\langle jm'|\exp(-\frac{i\beta}{\hbar}J_y)|jm\rangle\exp(-i\gamma m) \end{aligned}$$

$$-i\beta J_y|\frac{1}{2}\frac{1}{2}\rangle = -\frac{\beta}{2}(J_+ - J_-)|\frac{1}{2}\frac{1}{2}\rangle = \frac{\beta}{2}|\frac{1}{2} - \frac{1}{2}\rangle$$

$$(-i\beta J_y)^2|\frac{1}{2}\frac{1}{2}\rangle = -(\frac{\beta}{2})^2(J_+ - J_-)|\frac{1}{2} - \frac{1}{2}\rangle = -(\frac{\beta}{2})^2|\frac{1}{2}\frac{1}{2}\rangle$$

$$(-i\beta J_y)^3|\frac{1}{2}\frac{1}{2}\rangle = -(\frac{\beta}{2})^3|\frac{1}{2} - \frac{1}{2}\rangle$$

$$(-i\beta J_y)^4|\frac{1}{2}\frac{1}{2}\rangle = (\frac{\beta}{2})^4|\frac{1}{2}\frac{1}{2}\rangle$$

Remembering $\exp(-\frac{i}{\hbar}\beta J_y) = \sum_{k=0}^{\infty}\frac{(-\frac{i}{\hbar}\beta J_y)^k}{k!}$ we see

$$\begin{aligned} \exp(-\frac{i}{\hbar}\beta J_y)|\frac{1}{2}\frac{1}{2}\rangle &= \sum_{k=0}^{\infty}\frac{(-1)^k(\frac{\beta}{2})^{2k}}{2k!}|\frac{1}{2}\frac{1}{2}\rangle + \sum_{k=0}^{\infty}\frac{(-1)^k(\frac{\beta}{2})^{2k+1}}{(2k+1)!}|\frac{1}{2} - \frac{1}{2}\rangle \\ &= \cos(\frac{\beta}{2})|\frac{1}{2}\frac{1}{2}\rangle + \sin(\frac{\beta}{2})|\frac{1}{2} - \frac{1}{2}\rangle \end{aligned}$$

and using the same approach

$$\exp(-\frac{i}{\hbar}\beta J_y)|\frac{1}{2} - \frac{1}{2}\rangle = -\sin(\frac{\beta}{2})|\frac{1}{2}\frac{1}{2}\rangle + \cos(\frac{\beta}{2})|\frac{1}{2} - \frac{1}{2}\rangle$$

and we have for the full matrix

$$D^{(1/2)}(\alpha\beta\gamma) = \begin{pmatrix} \exp(-i(\alpha+\gamma)/2)\cos(\beta/2) & -\exp(i(\gamma-\alpha)/2)\sin(\beta/2) \\ \exp(i(\alpha-\gamma)/2)\sin(\beta/2) & \exp(i(\alpha+\gamma)/2)\cos(\beta/2) \end{pmatrix}$$

We noticed before that the Wigner function $D^{(j)}_{m'm}$, *i.e.* the matrix elements of the rotation operator $D(\omega)$ is often referred to as the $2j+1$-dimensional irreducible representation of the rotation operator $D(\omega)$. We realize that the matrix which correspond to an arbitrary rotation operator can be brought to block-diagonal form, *i.e.*

$$\begin{pmatrix} \begin{pmatrix} x & x \\ x & x \end{pmatrix} & & \\ & \begin{pmatrix} x & x & x \\ x & D^{(j)}_{m'm} & x \\ x & x & x \end{pmatrix} & 2j+1 \\ & 2j+1 & \begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{pmatrix} \end{pmatrix}$$

Note that each smaller matrix can not be reduced further. Also note that $D^{(j)}$ form a group because

i) $\theta = 0$ means that 1 is a member of the group.
ii) $\theta \to -\theta$ means that the inverse is a member
iii) It is not possible to multiply oneself out of the group, *i.e.* any two rotations can be replaced by a single rotation.
iv) The rotation matrix is unitary.

To exemplify the above discussion we investigate what happens to the product function

$$|\gamma_1 j_1 m_1\rangle|\gamma_2 j_2 m_2\rangle \tag{3.21}$$

under a rotation

$$D(\omega)|\gamma_1 j_1 m_1\rangle|\gamma_2 j_2 m_2\rangle = \sum_{m_1 m_2})|\gamma_1 j_1 m_1'\rangle|\gamma_2 j_2 m_2'\rangle D^{(j_1)}_{m_1' m_1} D^{(j_2)}_{m_2' m_2} \tag{3.22}$$

Thus the product function transform according to the direct product of the two representation matrices $D^{(j_1)}$ and $D^{(j_2)}$. We have a new representation $D^{(j_1)} \times D^{(j_2)}$. Note that this is a "super matrix" with the elements $(A \times B)_{il,km} = A_{ik}B_{lm}$ if the elements of A and B are A_{ik} and B_{lm}, respectively.

We also know that using

$$|\gamma j_1 j_2 JM\rangle = \sum_{m_1+m_2=M} |\gamma j_1 j_2 m_1 m_2\rangle\langle\gamma j_1 j_2 m_1 m_2|\gamma j_1 j_2 JM\rangle \tag{3.23}$$

we can form a linear combination of the product function $|\gamma j_1 j_2 m_1 m_2\rangle$ that transform according to $D^{(J)}(\omega)$, *i.e.* $D^{(j_1)} \times D^{(j_2)}$ is reducible to block-diagonal form, the number of basis functions have been reduced!

Before starting our discussion on tensor operators we note that there exist an explicit formula for the general matrix element of the rotation operator, namely

$$\langle JM'|D(\omega)|JM\rangle = D^{(J)}_{M'M}(\omega) = \exp(-i(\alpha M' + \gamma M))\langle JM'| - i\beta J_y \hbar|JM\rangle \tag{3.24}$$

where

$$\begin{aligned} \langle JM'| - i\beta J_y\hbar|JM\rangle &= \sum_t (-1)^t \frac{t((J+M')!(J-M')!(J+M)!(J-M)!)^{1/2}}{(J+M'-t)!(J-M-t)!t!(t-M-M')!} \\ &\times \ (\cos\frac{\beta}{2})^{2J+M'-M-2t}(\sin\frac{\beta}{2})^{2t+M-M'} \end{aligned} \tag{3.25}$$